Indian J. Phys. **51A**, 1-6 (1977)

Some non-resonance excitations of Na by electrons : Application of combined classical theory.

D. N. Roy

Department of Physics, Patna University, Patna-800005

(*Received* 3 *February* 1976)

Percival's combined classical theory (1973) has been extended to include the case of eccentricity equal to one and applied to calculate 4s, 5s and 6s excitation cross-sections from the ground state of Na atom by electron impact. The results are found to be in better agreement with experimental results than those of the combined theory for micro-canonical distribution and also the First Born approximation.

1. Introduction

Classical theories, despite their wellknown inadequacies have proved useful in the study of inelastic collisions of atoms by charged particles. Analytic classical theories of atomic excitations are (*i*) binary encounter theory (Gryzinski 1965, Vriens 1966) and (*ii*) dipole perturbation or adiabatic theory (Percival *et al* 1967). While the binary encounter theory is valid for large energy transfers, the dipole perturbation theory is valid for small energy transfers only. Recently (1973) Percival has presented a classical theory of excitation valid for adiabatic intermediate and impulsive collisions for all energy transfers subject to the condition that incident energy is sufficiently large. He has shown that the binary encounter theory and the adiabatic theory are the limiting forms of this *combined* theory. Percival has developed the theory for circular orbits (eccentricity $\epsilon = 0$) and microcanonical distribution of orbits. Gryzinski (1973) has criticized the use of microcanonical distribution for ground state of hydrogen and has suggested instead the free fall model ($\epsilon = 1$). Assuming in this light that the ground state of the alkali atoms are better described by the eccentricity one than the microcanonical distribution, we have developed, following Percival, the combined theory for $\epsilon = 1$. In this paper we have presented the theory for $\epsilon = 1$, tabulated the cross-section function $C_1(q)$ and approximated it by a simple form. Then we have produced the results of this theory applied to some excitations of Na atom. For comparison we have also calculated the cross-sections assuming microcanonical distribution using the analytic form suggested by Percival. We have also compared these results with the available experimental data and other theoretical results.

2. Theory

Following Percival (1973) the differential cross-section is given by

$$\frac{d\sigma}{d\Delta E} = \frac{\pi a^2}{U} \left| \frac{Z_3}{Z_1} \right| \left(\frac{m E_1}{2m_1 U} \right)^2 |C(\boldsymbol{q}_-)-C(\boldsymbol{q}_+)|. \quad \dots (1)$$

where a is the semi-major axis of classical atom, U is the ionization energy, Z_1e and m_1 are the charge and the mass of the incident particle. m_e the mass of the bound electron, Z_3e is the charge of the nucleus. $\boldsymbol{q}$ is the dimensionless momentum transfer equal to q/q_{ad} where

$$q_{ad} = \frac{|4Z_1e^2\omega|}{2v_1^2}$$

The two limits on the momentum transfer are defined by

$$\boldsymbol{q}_{\pm} = \left| \frac{Z_3}{Z_1} \right| \left(\frac{m_e E_1}{2m_1 U} \right) \left[\left(1+\frac{\Delta E}{U} \right)^{\frac{1}{2}} \pm 1 \right] \quad \dots (2)$$

where $U = Z_3e^2/2a$ has been used.

For electron incident on neutral Na, Z_3e is the effective charge of the nucleus for the bound electron and $m_e = m_1$. Therefore the two equations reduce to

$$\frac{d\sigma}{d\Delta E} = \frac{\pi a^2}{U} \left| \frac{Z_3}{Z_1} \right| \left(\frac{E_1}{2U} \right)^2 [C(\boldsymbol{q}_-)-C(\boldsymbol{q}_+)] \quad \dots (3)$$

$$\boldsymbol{q}_{\pm} = \left| \frac{Z_3}{Z_1} \right| \left(\frac{E_1}{2U} \right) \left[\left(1+\frac{\Delta E}{U} \right)^{\frac{1}{2}} \pm 1 \right]. \quad \dots (4)$$

The cross-section function $C(\boldsymbol{q})$ stands for the integral

$$C(\boldsymbol{q}) = \int_0^b \frac{\boldsymbol{b}d\boldsymbol{b}}{\boldsymbol{q}} \quad \dots (5)$$

where $\boldsymbol{b} = b/b_{ad}$ is the dimensionless impact parameter. Integral (5) is evaluated by numerical integration with the helpo f the functiona relation between $\boldsymbol{q}$ and $\boldsymbol{b}$.

$$\boldsymbol{q}(\boldsymbol{b}) = \left\{ \sum_{s=1}^{\infty} 2s^2 M_s [K_0^2(s\boldsymbol{b})+K_1^2(s\boldsymbol{b})] \right\}^{\frac{1}{2}} \quad \dots (6)$$

where $M_s = \{J_t'(s)\}^2$. J and K are respectively ordinary and modified Bessel functions.

2. Results

The cross-section function $C(q)$ were calculated by numerical integration using Simpson's rule and have been tabulated in table 1 for the relevant range of q. To obtain $C(q_{\pm})$ either the graphical method may be used or the approximate form

$$C_{AN}{}^{1}(q) = \frac{x^2}{4+2\cdot 2x}\ln(1+0\cdot 75x); \quad x = 1/q \qquad \ldots \quad (7)$$

may be used. This approximate form is in some interval of q (as shown in table 1) as much as 13% in error. The calculated value was corrected by the appropriate factor. In $3S \to 4S$ excitation graphical method was used which may be in error by about 5%. In other excitations the analytic form eq. (7) was used which reduced the error to about 1%.

Table 1. Values of the C-function for eccentricity one. $C_{AN}{}^{1}$ is the approx. form equation (7). $C_{BE} = 1/3q^3$ is the binary encounter C-function

b	q	$1/q$	b/q	$C_1(q)$	$C_{AN}{}^{1}$	$C_{AN}{}^{1}/C_1$	C_1/C_{BE}
0	∞	0	0	0			1
0·01	80·29	1·21(2)	1·24(- 4)	5·4 (- 7)			0·85
0·02	40·11	2·49(2)	1·98(4)	3·31(6)			0·65
0·03	26·64	3·75(2)	1·126(- 3)	1·13(– 5)			0·65
0·04	19·12	5·15(- 2)	2·06(3)	2·69(5)	2·44(– 5)	0·91	0·59
0·05	15·49	6·45(- 2)	3·23(– 3)	5·32(5)	5·28(- 5)	0·99	0·59
0·10	7·26	0·138	0·014	4·53(- 4)	4·36(– 4)	0·96	0·52
0·15	4·64	0·215	0·032	1·57(3)	1·54(– 3)	0·98	0·47
0·20	3·33	0·300	0·060	3·82(3)	3·91(3)	1·02	0·42
0·25	2·54	0·390	0·097	7·72(- 3)	8·02(3)	1·04	0·39
0·30	2·03	0·490	0·150	1·38(- 2)	1·47(– 2)	1·06	0·35
0·40	1·40	0·710	0·28	3·52(3)	3·86(2)	1·10	0·30
0·50	1·04	0·960	0·48	7·21(- 2)	8·17(2)	1·13	0·24
0·60	0·[illegible]4	1·245	0·75	0·133	0·151	1·13	0·21
0·70	0·639	1·564	1·095	0·225	0·255	1·13	0·18
0·80	0·52	1·92	1·54	0·355	0·400	1·13	0·15
1·0	0·36	2·78	2·78	0·779	0·861	1·10	0·11
1·2	0·26	3·87	4·64	1·51	1·63	1·08	0·08
1·4	0·19	5·26	7·36	2·69	2·84	1·06	
1·6	0·14	7·00	11·20	4·54	4·63	1·02	
1·8	0·11	9·21	16·57	7·27	7·23	0·99	
2·0	0·083	11·95	23·91	11·3	10·8	0·96	
2·2	0·065	15·43	33·95	17·0	15·9	0·93	
2·4	0·050	20·0	48·0	25·15	23·08	0·92	

Number in the parenthesis indicate the powers of ten with which the entries should be multiplied.

The last column shows that C_1/C_{BE} approaches 1 as q increases.

In the calculation of $q(b)$ from eq. (6), 20 terms have been used for very large q, while 10 terms have been used for lower values. For small q only 5 terms have been found enough, after which, terms become less than 1% of the leading term. The value of Z_3 used is 1·844. This is the value of Z_{eff} (effective charge) obtained from $T = RZ_{eff}{}^{2}/n^{2}$.

In table 2, the results of our calculations for $\epsilon = 1$ and micro-canonical distribution are given. For the latter calculations we used

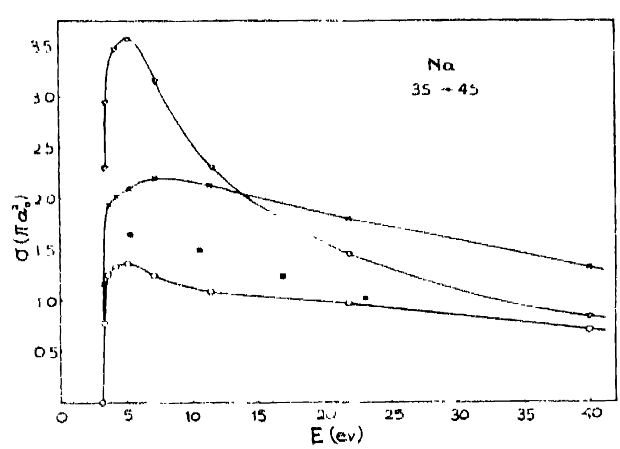
$$C_{AN}^{\mu}(q) = \frac{x^2}{2+3x/2}\ln(1+2x/3); \quad x = 1/q \qquad \ldots \quad (8)$$

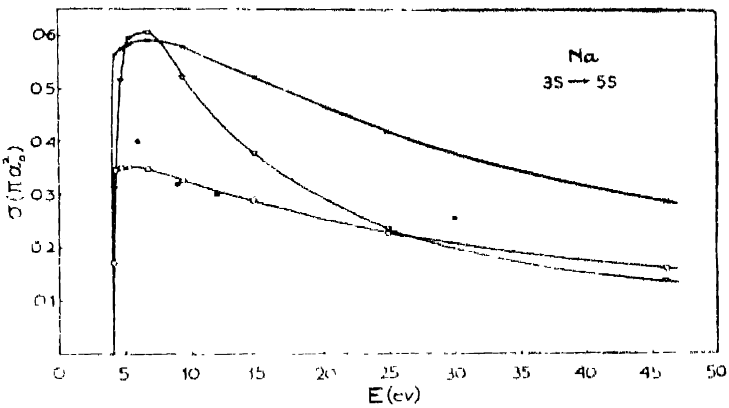
as suggested by Percival

Results have been graphically compared with the FBA calculations of Vainshtein *et al* as quoted by Moisewitsch *et al* (1968) and with the experimental results of Zapesochnsyi *et al* modified according to the suggestions of Moisewitsch *et al* (1968).

Table 2. Total excitation cross-sections for 4*s*, 5*s* and 6*s* excitations from the ground state of sodium by electron impact, calculated using $\epsilon = 1$, (σ_1) and microcanonical distribution, (σ_μ), in the combined classical theory

Energy in Threshold units	3*s*–4*s*		3*s*–5*s*		3*s*–6*s*	
	$\sigma_1(\pi a_0^2)$	$\sigma_\mu(\pi a_0^2)$	$\sigma_1(\pi a_0^2)$	$\sigma_\mu(\pi a_0^2)$	$\sigma_1(\pi a_0^2)$	$\sigma_\mu(\pi a_0^2)$
1·02			0·17	0·28	0·1502	0·2476
1·04			0·348	0·565	0·1504	0·2482
1·08	0·78	1·18	0·350	0·569	0·1508	0·2492
1·16	1·26	1·94	0·350	0·575	0·1512	0·2509
1·32	1·32	2·02	0·352	0·581	0·1497	0·2525
1·64	1·36	2·14	0·348	0·589	0·1450	0·2516
2·28	1·24	2·19	0·326	0·577	0·133	0·241
3·56	1·09	2·13	0·29	0·522	0·115	0·212
6·12	0·97	1·80	0·23	0·416	0·0914	0·163
11·24	0·71	1·32	0·16	0·286	0·0630	0·110
21·48	0·39	0·85	0·10	0·175	0·0378	0·0658





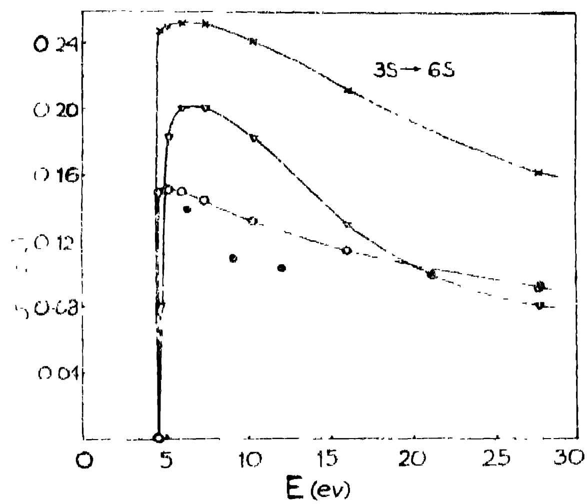


Fig 1 3s 4s, Figure 2 3s–5s and Figure 3 3s 6s excitation cross sections of Na by electrons

Solid line with circles: Combined theory with $c = 1$
Solid line with cross: Combined theory for microcanonical distribution
Solid line with triangles: First Born Approx. by Vainshtein *et al*
Circular dots: Modified experimental results of Zapesochnyi *et al*
Rectangular dots Modified results of close coupling approx by Korff *et al*

1. Discussion

The cross-section σ_1 for $c = 1$ is found always to be appreciably lower (a factor of $\frac{1}{2}$) than σ_μ, for microcanonical distribution. At lower energies the cross-sections σ_1 are lower than the first Born cross-sections but become comparable with Born cross-section at energies higher than about 20 ev. In 4s excitation, the close coupling calculations of Korff *et al* (1973), give nearly the same result as the First Born cross-sections. Korff *et al* have neglected exchange effects. They suggest that inclusion of exchange should reduce their cross-section by 10% at 10·5 ev and about 30% at 16·8 ev. Their values modified by this prescription reduce to $\sim 1{\cdot}5\ \pi a_0^2$ at 10·5 ev and $\sim 1{\cdot}25\ \pi a_0^2$ at 16·8 ev. These values are only about 25% higher than σ_1. The maximum of the cross-section obtained experimentally by Zapesochnyi *et al* when modified by the prescription of Moisewitsch and Smith (1968) is $\sim 1{\cdot}63\ \pi a_0^2$ at 5·3 ev incident energy. σ_1 has maximum at almost the same point with a value which is about 16% lower than this experimental result.

In 5s and 6s cross-sections also the maximum value of σ_1 compares favourably with the experimental results of Zapeschonyi and Shimon (modified value taken from Massey & Burhop (1969). In the former our value is only 12% lower and in the latter 9% higher than the corrected experimental value. However the location of the peak is at slightly lower incident energy than the experimental value.

5. Conclusion

Our results confirm that the ground state of an alkali atom, atleast for the purposes of this theory, is better represented by the "free fall model" than the microcanonical distribution. Further it appears that the combined classical theory can give reliable results even at low energies for excitations to higher levels. In view of the meagre experimental results available and the difficult quantum mechanical calculations this simple method can be very useful for those working in astrophysics or plasma physics and needing a good estimate of the excitation cross-section. We expect that inclusion of exchange will further improve the results.

Work is being continued to include exchange and also to apply this theory to other atomic and ionic excitations to test the efficiency of the theory.

Acknowledgment

I am grateful to Prof. L. S. Singh of the Department of Physics, Patna University for suggesting the problem and continued guidance throughout the progress of the work.

References

Gryzinski M. 1965 *Phys. Rev.* 138 **2A**, 335.

Gryzinski M., Kune J., & Zgorzelski M. 1973 *J. Phys. B. Atom Molec Phys.* **6**, 2292.

Korff D. F. Chung S. & Lin C. C. 1973 *Phys. Rev.* **A7**, (2) 545.

Massey H. S. W. & Burhop E. H. S. 1969 *Electronic & Ionic Impact Phenomena* Vol. I, p. 226, Oxford Press.

Moisewitsch B. L. & Smith S. J. 1968 *Rev. Mod. Phys.* **10**(**2**), 238

Percival I. C. 1973 *J. Phys. B. Atom Molec. Phys.* **6**, 2236.

Percival I. C. & Richards S. 1967 *Proc. Phys. Soc.* **92**, 311.

Vriens L. 1966 *Phys. Rev.* **141**, 88.